

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 31.7 °C

Global applicability domain: Inside

Local applicability domain index: 5.98e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Cycloate</div> <div>Measured: 11.5</div> <div>Predicted: 31.7</div>	<div>Image not found</div> <div>Methsuximide</div> <div>Measured: 52.5</div> <div>Predicted: 68.0</div>	<div>Image not found</div> <div>Phensuximide</div> <div>Measured: 72.0</div> <div>Predicted: 77.2</div>
<div>Image not found</div> <div>N-Ethylphthalimide</div> <div>Measured: 79.0</div> <div>Predicted: 82.4</div>		